

7,7'-(Carbonyldiimino)bis[4-hydroxy-2-naphthalenesulfonic acid]
134-47-4 | DTXSID7059642

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.38e-03 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.19e-01

Confidence level: 4.99e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methacycline</div> <div>Measured: 1.71e-02</div> <div>Predicted: 2.27e-03</div>	<div>Image not found</div> <div>Tetracycline</div> <div>Measured: 5.20e-04</div> <div>Predicted: 2.23e-03</div>	<div>Image not found</div> <div>Doxycycline</div> <div>Measured: 1.42e-03</div> <div>Predicted: 2.24e-03</div>
<div>Image not found</div> <div>Minocycline</div> <div>Measured: 1.14e-01</div> <div>Predicted: 4.97e-03</div>	<div>Image not found</div> <div>Demeclocycline</div> <div>Measured: 3.26e-03</div> <div>Predicted: 2.24e-03</div>	